

# Discussion session : pseudos

A real lack : systematic approach to provide reliable pseudopotentials/PAW datasets for ABINIT.

Description of the current status of abinit/psps project ...  
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- The long- and medium-term objectives, components, and strategy (XG)
- The repositories and database components (AJ)
- A tool for the comparison of output files (DW)
- Validating : comparison between ELK and ABINIT (MS)



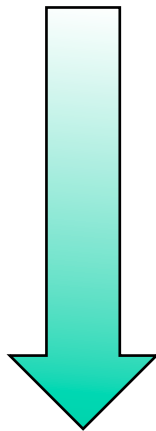
# abinit/psps project

Global long-term objectives :

G1. To have, on the Web, sets of **validated** pseudopotentials for **the whole periodic table**, for **different XC**, for **diff. #el** (semi-core), for **diff. cut-off radii**, with optimal ecut

G2. To have **a Web portal** for the generation/validation of new pseudos

Intermediate objectives, more and more difficult :



- (1) Robust, automatic **generation** of one pseudopotential
- (2) Automatic **computation** of selected physical properties for the pseudo (atom/dimer/elemental solid/oxyde)
- (3) Automatic **validation** with respect to a reference
- (4) Automatic **improvement** of the generation of pseudo (e.g. optim ecut)
- (5) Automatic **generation of a set of pseudopotentials**

+ development of Web tools, and building of the hardware resources



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Strategy ...

Components : repositories ; data structure ; software ; hardware.

For the datastructure and software components, place them under version management, with easy worldwide access, automatic testing.

Repositories and data structure :

- bzt (the structure is already set up)

bzt+ssh://psps@archives.abinit.org/forge/psps/001-H

...

bzt+ssh://psps@archives.abinit.org/forge/psps/008-O

...

bzt+ssh://psps@archives.abinit.org/forge/psps/014-Si

...

bzt+ssh://psps@archives.abinit.org/forge/psps/bin

bzt+ssh://psps@archives.abinit.org/forge/psps/share

+ abinit/psps/README, abinit/psps/scripts, abinit/psps/tests

cd abinit/psps ; bzt branch bzt+ssh://psps@archives.abinit.org/forge/psps/014-Si



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Software / Hardware ... in progress

- of course, ATOMPAW, ABINIT, ELK and drivers ;
- going from CIF file to ABINIT/ELK input file ;
- comparison of output files ;
- gathering of data from output files in database
- ...
- buildbot + a farm of machines
- optimizer

Gradual understanding of the CPU constraints, memory constraints and human time needed.

Adjust the objectives to stay realist

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